

**OPTIMAL LINEAR/NONLINEAR QUANTITY/QUALITY MANAGEMENT
FOR COMPLEX MULTILAYER AQUIFERS BY EMBEDDING**

by Ali Gharbi and Richard C. Peralta

Department of Biological and Irrigation Engineering
and

International Irrigation Center

Utah State University
Logan, UT 84322-4105
(801) 750-2785
FAX (801) 750-1248

Table of Contents

Abstract	1
Introduction	1
Terms Definitions	4
Planning Period and Stress Period	4
Iteration and Cycle	4
Model Formulation	5
Objective Formulation	5
Constraints	5
Finite-difference Approximation of the Flow Equation	5
The 2-D Galerkin-finite-element Approximation of the Unsteady State Solute Transport	6
Over and Under Achievement Values for Concentrations	8
Expressions Describing Evapotranspiration	8
Expressions Describing the Stream-aquifer Interflow	10
Expression Describing the General-Head Boundary	11
Constraint on Stream-aquifer Interflow for Each Reach	11
Expressions Describing Flow Reduction	11
Expressions Describing Drain-aquifer Interflow	12
Monotonocity and Sustainability Constraint	13
Bounds	13
Solution Using Linear and Nonlinear Model Options	14
Linear Model	14
Nonlinear Model	14
USUEM's Integrated Modeling Structure	14
Integrated Approach Solution Technique	15
Switching between Linear and Nonlinear options	16
Linear option	16
Nonlinear option	17

Table of Contents (cont.)

Numerical Difficulties and Possible Solutions	17
Solver Declares Problem To Be Infeasible	17
Other Difficulties	18
Summary and Conclusions	18
Summary	18
Conclusions	20
Notations	25
References	30

List of Figures

Figure 1.	Description of a Cycle	22
Figure 2.	Man/Machine Decision Tree for Computing Optimal Solution Using USUGWM	23
Figure 3.	Overview of Data Input, Model Construction, Solution Process, and Modules Called	24

OPTIMAL LINEAR/NONLINEAR QUANTITY/QUALITY MANAGEMENT OF COMPLEX MULTILAYER AQUIFERS BY EMBEDDING

A. Gharbi

Agricultural and Irrigation Engineering Department, Utah State University

R.C. Peralta

Agricultural and Irrigation Engineering Department, Utah State University

The embedding optimization modelling approach is adapted to aid long-term groundwater quality and quantity management of complex nonlinear multilayer aquifers. Implicit block-centered finite-difference approximations of the quasi-three-dimensional unsteady flow equation, and Galerkin finite-element approximations of the two-dimensional advection-dispersion transport equation are embedded as constraints in the model. Other hydrological processes are also included as constraints. Cyclical linear differencing permits representation of nonlinear transport, even when contaminant is extracted by unsteady pumping (a decision variable). Also used are nonlinear (discontinuous derivative) constraints describing drainage, stream-aquifer interflow and evapotranspiration. The use of both linear and nonlinear formulations of the entire flow and transport model in a cyclical manner reduces execution time and improves confidence in solution optimality. The resulting model incorporates the dynamic changes in parameters characterizing nonlinear groundwater systems. The methodology is most suitable for reconnaissance planning in nonlinear systems typified by: (1) relatively large cell size, (2) large proportion of the cells having head-dependent external fluxes and pumping decision variables, and (3) the need for dispersed contaminant management. It uses a multiobjective weighting approach and goal programming to maximize sustainable groundwater extraction while achieving target groundwater concentrations in control nodes. In a second paper, the methodology is applied to the Salt Lake Valley.

1. Introduction

Several models dealing with optimizing groundwater quantity and quality management have been previously reported. Assumptions regarding system linearity were commonly used to justify the use of both the response matrix and the embedding approaches. These assumptions are justified in most reported cases, and are especially adequate when the constraint equations are continuous and differentiable. However, formulations of stream-aquifer interflow, evapotranspiration (E_t), and flow from drains can be nonsmooth and not continuously differentiable. In addition, solute movement in initially unknown unsteady flow fields when solute is being extracted by pumping is nonlinear. In such cases, normal assumptions of linearity can become inappropriate and the response matrix approach cannot be applied (Willis and Jones, [1987]), without

modification.

Gorelick et al. [1984] presented a methodology to address the nonlinearity in the flow and transport equations when the response matrix is used. Their approach was based upon the governing equations for steady state confined areal groundwater flow, and areal non reactive solute transport. They used a simulation model SUTRA (Voss, [1983]) to compute the Jacobian of the nonlinear constraints (transport equation) with respect to each decision variable (pumping or injection) after each iteration. This Jacobian and other constraints are used as linear constraints for a subsequent optimization model. Ahfeld et al. [1986] tested the same procedure on a hypothetical system of 100 nodes. They considered the steady state formulation for the flow and a transient regime for the transport. A total of 12 3-month time steps were considered. They concluded that computational costs are dominated by the repeated simulations required to compute the Jacobian and that this characteristic limits the use of this methodology to problems with few decision variables. In their results, CPU time ranges from 0.51 hours for 5 pumping wells and 12 observation wells to 70 hours for 35 pumping wells and 70 observation wells. More than 90% of the CPU time is spent in the simulations. To avoid the repeated computation of the Jacobian matrices after each iteration, Ahfeld et al. [1988] used sensitivity theory to derive a general relationship for computing each element of the Jacobian. Their approach reduced the number of necessary simulations, and reduced execution time. Danskin and Gorelick [1985] used a similar approach.

In spite of the rapid improvement in computer availability (speed and memory) there have been few recent attempts to improve the embedding approach for solute transport management. This despite the fact that the embedding technique is widely acknowledged to be easier to understand and formulate. Until now, the embedding approach has been considered to be especially suitable for cases of steady state flow in which a large proportion of cells had pumping or flow decision variables and many cells needed head constraints. In such cases, the response matrix approach requires very large matrices to describe the effects of unit pumpings on each constrained cell.

Willis [1979] used the embedding technique to develop a model for the management of groundwater quality. The Galerkin finite-element method was used to approximate both flow and transport equations. The model was then decomposed into two independent subproblems and solved using linear programming.

Peralta and Killian [1985] included the steady flow equation in their optimization to develop regional optimal potentiometric surfaces. Datta and Peralta [1986] used the surrogate worth trade-off method with the embedding technique in regional sustained groundwater yield planning. Peralta and Killian [1987] solved a multi-objective problem using the embedding technique for a region containing of 254 cells. Peralta and Datta [1990] optimized perennial yield planning for a 3,200 square mile area of over 300 cells. In all of those efforts, all cells were pumping cells, each cell contained numerous wells. Linear systems were assumed.

Yazicigil and Rasheeduddin [1987] used the embedding technique to solve for a two-layered system under unsteady state conditions. They considered sixty cells and 4 time steps, with possible pumping from 18 cells. Cantiller et al. [1988] used the

embedding technique in optimizing conjunctive use of surface water and sustained groundwater pumping for eastern Arkansas.

Willis et al. [1989] developed a model for water quantity management in North China Plain. He included the finite element approximation of the flow equation as a constraint. His model consisted of 298 nodes for 247 elements, to cover a surface of about 190,000 hectares. A total of 594 pumping wells were considered.

Nevertheless, several researchers have reported difficulties with using the embedding method, especially for transient conditions [Aguado and Remson, 1974; Gorelick, 1983; Evans and Remson, 1982; Elango and Rouve, 1980; Tung and Kolterman, 1985; and Yazdanian and Peralta, 1986]. Some suggested that without the improvement of used optimization algorithms, the embedding method should be dropped in favor of the "response matrix approach". They noticed that the main reason was the unavailability of commercial solution routines for large linear programming problems similar to those encountered in large scale water management projects. The routines they used had difficulties with lower-upper basis factorization when banded matrices are involved, which led to numerical instability. Cantiller et al. [1988] were able to circumvent that problem using MINOS, an optimization algorithm (Saunders and Murtagh, [1985]), however they still assumed system linearity.

Ahfeld (1990) stated that because of the unavailability of adequate technology to address the remediation problem, hydraulic control methods can help contain groundwater contaminants. Therefore, they developed a two stage groundwater design for systems that can reach rapidly their steady state regime.

Dougherty and Marryot [1991] applied the simulated annealing methodology to groundwater management. They concluded that further testing and improvements can be expected. Culver and Shoemaker [1992] used the SALQR (successive approximation linear quadratic regulator) method for groundwater remediation. They used different time steps for both the optimization model and the numerical groundwater model.

This paper presents a procedure that overcomes difficulties previously associated with using the embedding method. It shows an integrated way of implementing the embedding method for optimizing pumping and groundwater quality management in complex aquifer systems having unsteady nonlinear flow and transport. To aid implementation, the method is contained within an interactive program. Included contributions are a linearized flow and transport model, a nonlinear flow and transport model, and, as is described later, partitioned and combined forms of the flow equation for both the linear and nonlinear models. The presented linear cyclical differencing approach permits optimizing unsteady pumping, while extracting contaminated water from cells at which pumping, concentration and head are all variables.

The presented method is useful for large scale, long term reconnaissance level planning. It is assumed that pumping in all wells in a cell can be adequately described by a single distributed pumping value in that cell and that heads and dispersed contaminant concentrations can be adequately represented by a single value in each cell.

The presented method is suitable for situations in which the embedding method is commonly preferred--systems in which a large proportion of the cells have pumping decision variables or require head constraints. It is also appropriate for reconnaissance

planning if a large proportion of the cells have nonsmooth variable-head dependent functions to describe flow processes.

To describe the methodology in an orderly fashion, some terms are defined first. Then is a description of the optimization model's objective function and constraints. Both linear and nonsmooth (nonlinear) forms of the constraints are shown. Included is linearization of advective transport via cyclical linear differencing. This is followed by an overview of the structure of the Utah State Univ. Embedding Model (USUEM), which integrates all the solution approaches. USUEM permits selecting solution approaches best suited for a particular problem. One discussed option is selecting linear versus nonlinear equation forms. Another option involves using separate equations, and variables, for each individual flow process (Et, flow to drains, stream/aquifer interflow) versus using a single flow equation and incorporating only heads and pumping as variables. Advantages and potential difficulties of the integrated solution method are highlighted, followed by summarization and conclusion. A companion paper demonstrates application to the Salt Lake Valley, a complex hydrogeological site.

It is important to note that, if better equations are available to describe any of the phenomenon that will be described in the following, the model can be modified easily.

2. Terms Definitions

2.1. *Planning Period and Stress Period*

In this model a stress period is defined as the time interval during which all external stresses such as pumping are constant. The planning period is the time interval during which the system is studied. The planning period is divided in a number of stress periods of equal or different lengths. For improved simulation accuracy, one can divide a long period of constant pumping into several shorter stress periods. This follows closely the terminology of MacDonald and Harbaugh [1984] in their MODFLOW model.

2.2. *Iteration and Cycle*

The term iteration refers to processing within the MINOS solver. All equations comprising the optimization model are solved during a particular iteration. Many iterations are usually required before MINOS halts computation and declares that an optimal solution is found. However, when addressing a nonlinear problem using a linear surrogate, that optimal solution might not be the best stopping point. Thus, after reinitialization, another optimization (cycle) might be performed. Many cycles might be needed before a satisfactory optimal solution is found. The general procedure is as follows (Fig. 1).

(1) A cycle for addressing an unconfined aquifer begins when assumed values (such as heads) are read. (2) Some parameters (such as transmissivities, and dispersivities) are then computed, and automatically placed within the optimization model

constraint equations. (3) Optimization begins and iterations are performed until an optimal solution is determined. (4) Then optimal strategy results (fluxes and heads) are compared with the values assumed in step (1). If the differences are acceptably small, the process halts. Otherwise, optimal strategy results are used in step (1) and a new cycle commences. Multiple cycles are usually needed to reach a satisfactory (converged) optimal solution for unconfined aquifers or systems having nonsmooth functions (discontinuous derivatives).

3. Model Formulation

3.1. Objective Function

Verbally, the multiple objectives used in this model involve maximizing Z , the total ground-water extraction, while minimizing the excessive groundwater contaminant concentrations during a planning period of K time steps. In a system of M total cells, Ω are cells where pumping is optimized, and NQ are nodes where water quality is to be controlled. This objective function uses the weighting approach to address noncommensurate multiple objectives.

$$\text{Max } Z = \sum_{k=1}^K \sum_{\omega=1}^{\Omega} g_{\omega,k} - wc \sum_{kq=1}^{KQ} \sum_{nq=1}^{NQ} c_{nq,kq}^+ \quad (1)$$

Where:

$g_{\omega,k}$ = spatially distributed pumping (+) from cell ω , during stress period k , [L^3T^{-1}]; Ω = total number of possible pumping cells in the study area; NQ = total number of nodes where water quality control is required; wc = weighting factor associated with quality control (When wc is equal to 0, the mono-objective is to maximize pumping. A large value of wc will force $c_{nq,kq}^+$ to be smaller), [$L^6M^{-1}T^{-1}$]; kq = time step used for water quality simulation (frequently one uses several smaller time steps for water quality simulation within one stress period used for flow simulation), [T]; $c_{nq,kq}^+$ = concentration in excess of the target concentration desired for node nq by the end of time step kq , [ML^{-3}]. Pumping, g , in studies such as this usually represents the total pumping of many individual wells within a cell. The resulting computed head is simply the representative value for the center of the cell, and does not reflect head at any particular well.

3.2. Constraints

3.2.1. Finite-difference Approximation of the Flow Equation

The optimization model contains as constraints an implicit quasi 3-D finite-difference approximation of the flow equation. To facilitate model verification and transferability, these constraints follow the block-centered approach of McDonald and Harbaugh [1988]. For a system of I rows, J columns and L layers, the flow equation can be represented by

$$f(h, \Delta x_j, \Delta y_i, \Delta z_l, T) = \frac{S_{i,j,l} \Delta x_j \Delta y_i}{\Delta t_k} (h_{\bar{o},k} - h_{\bar{o},k-1}) + q_{\bar{o},k}^b + q_{\bar{o},k} \quad (2)$$

$$+ q_{\bar{o},k}^s + q_{\bar{o},k}^c + q_{\bar{o},k}^p \quad \text{for } \bar{o} \in M, k \in K$$

Where \bar{o} is the number of a particular cell (i,j,l) located in row i , column j and layer l ; $T_{i,j,l}$ = transmissivity for cell (i,j,l) , $[L^2T^{-1}]$; $h_{i,j,l,k}$ = potentiometric head for cell i,j,l , at the end of time step k , $[L]$; $S_{i,j,l}$ = storage coefficient or specific yield for cell i,j,l ; $\Delta x_j, \Delta y_i, \Delta z_l$ = cell size in x , y and z directions, of cell \bar{o} , $[L]$; Δt_k = duration of time step k , $[T]$; $h_{\bar{o},k}$ = average potentiometric head in cell \bar{o} at end of stress period k , $[L]$; $q_{\bar{o},k}^b$ = known flow across the boundaries of the study area (i.e., bedrock recharge that is not a function of head, $[L^3T^{-1}]$; $q_{\bar{o},k} = g_{\bar{o},k} + q_{\bar{o},k}^d + q_{\bar{o},k}^t + q_{\bar{o},k}^z$; $q_{\bar{o},k}^d$ = distributed discharge from (+) or recharge to (-) the aquifer in cell \bar{o} in stress period k , that is a function of ground water or surface water management, $[L^3T^{-1}]$; $q_{\bar{o},k}^t$ = distributed evapotranspiration (+) or recharge by accretion (-) to the aquifer in cell \bar{o} and time step k , $[L^3T^{-1}]$; $q_{\bar{o},k}^z$ = lateral flow across a boundary (which depends on the boundary's fixed head and adjacent heads), $[L^3T^{-1}]$; $q_{\bar{o},k}^s$ = flow between the aquifer and streams, $[L^3T^{-1}]$; $q_{\bar{o},k}^d$ = flow from the aquifer to drains (+), $[L^3T^{-1}]$; $q_{\bar{o},k}^c$ = saturated flow between the aquifer and general head boundary cells, $[L^3T^{-1}]$; $q_{\bar{o},k}^p$ = reduction in vertical flow between cells in layer l and the lower layer $l+1$ due to drop in head below the top of layer $l+1$, $[L^3T^{-1}]$; and $f(h, \Delta x_j, \Delta y_i, \Delta z_l, T)$ is the finite-difference form of the unsteady state quasi 3-D flow equation as well described by McDonald and Harbaugh [1988].

3.2.2. The 2-D Galerkin-finite-element Approximation of the Unsteady State Solute Transport

The basic form of the finite element transport equation embedded as constraints in the optimization model is similar to that outlined by Huyakorn [1986] for simulation, except that the consistent formulation is used instead of the lumped form when approximating the time dependant term in the transport equation (Voss, [1984]).

The nonlinear formulation of the transport equation is:

$$(A_{nm} + \frac{D_{nm}}{\Delta t_{kq}}) c_{m,kq+1} = \frac{D_{nm}}{\Delta t_{kq}} c_{m,kq} + B_n \quad (3)$$

Where:

n and m = designators identifying individual nodes from among the N total finite-element nodes where concentrations are to be computed; e = a designator identifying one of the total of E elements; Δt_{kq} = duration of the time step kq , a fraction of Δt_k . This allows smaller time steps for the transport, $[T]$; $w(e)$ and $l(e)$ = the width and length of the rectangular element e , $[L]$;

$$\begin{aligned}
 A_{nm} = & \sum_{e=1}^E \langle D_{xx} \rangle^e \frac{w(e)}{l(e)} [A_D^{xx}]^e + \langle D_{yy} \rangle^e \frac{l(e)}{w(e)} [A_D^{yy}]^e \\
 & + \langle D_{xy} \rangle^e [A_D^{xy}]^e + \langle V_x \rangle^e \frac{w(e)}{2} [E_V^x]^e \\
 & + \langle V_y \rangle^e \frac{l(e)}{2} [E_V^y]^e - \frac{W(e)}{eb} \frac{L(e)w(e)}{36} [A_s]^{(e)}; \\
 D_{nm} = & [A_t]^e, \quad n \text{ and } m \in \text{element } e;
 \end{aligned} \tag{4}$$

$\langle V_x \rangle^e$, $\langle V_y \rangle^e$, $\langle D_{xx} \rangle^e$, $\langle D_{yy} \rangle^e$, $\langle D_{xy} \rangle^e$, $[A_D^*]^e$, $[E_V^*]^e$, $[A_t]^e$, $[A_s]^e$, and B_n are as well described by Huyakorn [1986].

In equation (3) the product of velocity, source or sink terms, and dispersivities constitute nonlinearities in the transport equation, since they are functions of initially unknown pumping and heads and are part of the solution.

Within the optimization model, it is desirable to have a linear means of expressing the transport process, even if pumping and flow fields are initially unknown. Here, this is done by separating the advection and dispersion processes and treating them as described below.

To linearly describe advective transport, the products of velocity, source or sink terms and concentrations in equation (4) are replaced by the following.

$$\begin{aligned}
 V c &= V_p c + V c_p - V_p c_p \\
 Q c &= Q_p c + V c_p - Q_p c_p
 \end{aligned} \tag{5}$$

where V_p , Q_p and c_p are respectively the velocity $[LT^{-1}]$, source or sink term $[L^3T^{-1}]$, and concentration $[ML^{-3}]$, from the previous cycle. Since values from a previous cycle are known in a subsequent cycle, each term in (5) has only one unknown and the equation is linear. This procedure reduced the nonlinearity that could otherwise make solution difficult.

Similarly, dispersivities are computed using known velocities from the previous cycle. Using equation (5) while cycling (which could be termed cyclical linear differencing), and using known velocities for dispersion greatly speed the process of converging to optimal solutions.

3.2.3. Over and Under Achievement Values for Concentrations

This constraint is intended to describe the computed concentration at a node with respect to a known reference concentration (target concentration).

$$C_{nq,kq} = C_{nq,kq}^{\text{target}} + C_{nq,kq}^+ - C_{nq,kq}^- \quad (6)$$

$$C_{nq,kq}^{\text{target}}, C_{nq,kq}^-, C_{nq,kq}^+ \geq 0$$

where $C_{nq,kq}^{\text{target}}$ = target concentration at node nq by the end of time step kq, $[ML^{-3}]$; $C_{nq,kq}^+$ = amount by which the concentration simulated for node nq by the end of time step kq exceeds the target concentration, $[ML^{-3}]$; $C_{nq,kq}^-$ = amount by which the optimal concentration is below the target concentration in node nq by the end of time step kq, $[ML^{-3}]$. Only one of the two achievement concentrations for a cell, C^+ and C^- , will be nonzero at the same time.

3.2.4. Expressions Describing Evapotranspiration

It is necessary to describe groundwater losses to the atmosphere resulting from evaporation and transpiration. The losses are functions of water table proximity to the ground surface (among other factors). Evapotranspiration can become significant in agricultural settings where irrigation and drainage are concerns. These are the same settings where the embedding model has been used the most for sustained groundwater yield planning (locations where most cells contain pumping as a decision variable).

Here and in sections 3.2.5-3.2.9, piecewise linear expressions used by USUEM are presented (these are similar to expressions in MODFLOW). Equivalent nonlinear equations are also shown. To facilitate solution, USUEM contains and uses both piecewise linear and the nonlinear expressions embedded as constraints, but not at simultaneously.

For clarity, the piecewise expressions are presented first. A piecewise constraint consists of more than one linear equation, each applicable within a certain range of values of water table elevation. Because of the abrupt transitions between linear segments, the total constraint equations are considered nonsmooth and their derivatives

are discontinuous.

In the piecewise evapotranspiration constraint below, three expressions are used to describe evapotranspiration response to water table head. A difficulty with using those constraints directly lies in the need to decide, before optimization, which linear segment to apply for each cell. Usually, one would pick the segment appropriate for the optimal head computed for that cell in the previous cycle. Unfortunately, segment preselection can cause fluxes and heads to change, causing the selected segment to differ from cycle to cycle. This flip-flopping can make convergence difficult. An alternative is to use the nonlinear form of the constraint. It is for this purpose that we developed the nonlinear representations of the piecewise constraints shown in this and subsequent sections.

- Piecewise linear evapotranspiration constraint:

$$\begin{aligned}
 q_{\bar{o},k}^t &= E_{\bar{o}} \Delta x_j \Delta y_i & \text{for } h_{\bar{s}_{\bar{o}}} < h_{\bar{o},k} \\
 q_{\bar{o},k}^t &= E_{\bar{o}} \Delta x_j \Delta y_i \frac{(h_{\bar{o},k} - (h_{\bar{s}_{\bar{o}}} - ds_{\bar{o}}))}{ds_{\bar{o}}} & \text{for } h_{\bar{s}_{\bar{o}}} - ds_{\bar{o}} < h_{\bar{o},k} \leq h_{\bar{s}_{\bar{o}}} \quad (7) \\
 q_{\bar{o},k}^t &= 0 & \text{for } h_{\bar{o},k} \leq h_{\bar{s}_{\bar{o}}} - ds_{\bar{o}}
 \end{aligned}$$

- Nonlinear evapotranspiration constraint.

$$q_{\bar{o},k}^t = \frac{E_{\bar{o}} \Delta x_j \Delta y_i}{ds_{\bar{o}}} (\min(h_{\bar{s}_{\bar{o}}}, h_{\bar{o},k}) - \min(h_{\bar{s}_{\bar{o}}} - ds_{\bar{o}}, h_{\bar{o},k})) \quad (8)$$

Where $E_{\bar{o}}$ = potential evapotranspiration in cell \bar{o} , [L]; $h_{\bar{s}_{\bar{o}}}$ = potentiometric surface elevation below which the evapotranspiration rate begins to decrease, [L]; $ds_{\bar{o}}$ = extinction depth in cell \bar{o} (depth below $h_{\bar{s}_{\bar{o}}}$ at which there is no evapotranspiration), [L], and $\min(r,s)$ is a function which equals the lesser numerical value of the expressions r and s .

In (8), the $\min(r,s)$ indicates that the model will, while performing the optimization, simultaneously select the smaller of r and s for use. It will do this even though the r and s expressions might both contain decision variables being optimized.

To illustrate interpretation of the $\min(m,n)$ function, first assume the case if $h_{\bar{o},k}$ is less than $(h_{\bar{s}_{\bar{o}}} - ds_{\bar{o}})$. (Obviously $h_{\bar{o},k}$ is also less than $h_{\bar{s}_{\bar{o}}}$.) The model will compute the portion of (8) in parentheses as $h_{\bar{o},k} - h_{\bar{o},k}$, or zero. Thus, the entire right hand side (RHS) will be zero. In other words, if the water table is low enough, evapotranspiration is zero.

If $h_{\bar{o},k}$ is greater than $h_{\bar{s}_{\bar{o}}}$ and $(h_{\bar{s}_{\bar{o}}} - ds_{\bar{o}})$, the part of the RHS in parentheses will equal $ds_{\bar{o}}$. Evapotranspiration loss will equal $E_{\bar{o}}$ times the cell area. Similarly, if its search for an optimal solution, the optimization model is changing $h_{\bar{o},k}$ from $h_{\bar{s}_{\bar{o}}}$ and $(h_{\bar{s}_{\bar{o}}} - ds_{\bar{o}})$

- ds_0), Et flux is changing linearly from a maximum rate to zero.

In essence, the $\min(r,s)$ function gives the model the ability to simultaneously determine variable values, while selecting appropriate equations for computing fluxes which are influenced by those variables. Without this ability in the optimization model, one would have to preselect which part of (7) to use. That preselection would affect the optimization process and might not even be correct for the resulting optimal solution. For example, one might assume that the water table will be low enough in one cell, due to pumping, that there will be no Et. If model constraints, such as a limit on acceptable drawdown at some other cell, prevents the water table from dropping in the first cell, Et should be computed. However, preselection of the wrong part of (7) will prevent the model from knowing that.

The nonlinear constraints described here and below are important for model performance because the potential errors caused by equation preselection can be significant in some situations. Such errors can result with other fluxes in addition to Et, for example, stream-aquifer interflow and flow from drains (surface or subsurface drainage systems). These three fluxes can account for half or more of the discharge from some systems.

3.2.5. Expressions Describing the Stream-aquifer Interflow

Stream-aquifer interflow is a complicated process. Many current publications still explore the interaction between aquifer and streams under different circumstances. In this paper, river stage is assumed constant during a stress period. This is a common assumption, especially in cases characterized by small variations in river stage (McDonald and Harbaugh, [1984]). A formulation was developed for cases where stage variation is considered. However it was not used due to the unavailability of stage/discharge data. Two different linear expressions can be applied, depending on the relation between the elevations of the aquifer water table and the bottom of the stream.

- Piecewise linear stream-aquifer interflow constraint:

$$\begin{aligned} q_{\bar{o},k}^s &= \Gamma_{\bar{o}} (h_{\bar{o},k} - \sigma_{\bar{o},k}) & \text{for } h_{\bar{o},k} \geq B_{\bar{o}} \\ q_{\bar{o},k}^s &= \Gamma_{\bar{o}} (B_{\bar{o}} - \sigma_{\bar{o},k}) & \text{for } h_{\bar{o},k} < B_{\bar{o}} \end{aligned} \quad (9)$$

- Nonlinear stream-aquifer interflow constraint:

$$q_{\bar{o},k}^s = \Gamma_{\bar{o}} \max(h_{\bar{o},k} - \sigma_{\bar{o},k}, B_{\bar{o}} - \sigma_{\bar{o},k}) \quad (10)$$

where $\Gamma_{\bar{o}}$ = hydraulic conductance of the stream-aquifer interconnection, (including any clogging layer), $[L^2T^{-1}]$; $\sigma_{\bar{o},k}$ = elevation of the free water surface in the river, $[L]$; $B_{\bar{o}}$ = bottom of the river in cell \bar{o} , $[L]$; $\max(r,s)$ equals the greater of the numerical values of the expressions for r and s .

Here, the nonlinear expression of $\max(a,b)$ performs as follows. If $h_{\bar{o},k}$ exceeds $\sigma_{\bar{o},k}$, a will be positive and b will be negative. Interflow will equal a positive discharge from the aquifer to the stream.

If $h_{\bar{o},k}$ is below $\sigma_{\bar{o},k}$ but above the base of the river, a will be negative but b will be even more negative. Thus the difference between groundwater level and river stage will drive the flow from river to aquifer.

If the groundwater table is below the base of the river, unsaturated flow is assumed. It is proportional to the difference between river stage and base elevations.

3.2.6. Expression Describing the General-Head Boundary

This constraint is similar to the one describing stream-aquifer interflow. It is applied to cases where saturated flow is considered to be always present.

$$q_{\bar{o},k}^c = \Gamma_{\bar{o}} (h_{\bar{o},k} - hc_{\bar{o},k}) \quad (11)$$

Where $hc_{\bar{o},k}$ = known potentiometric head for the general-head boundary in cell \bar{o} , $[L]$.

3.2.7. Constraint on Stream-aquifer Interflow for Each Reach

These bounds are used to limit or assure a certain stream-aquifer interflow. They are used to keep the model from inducing (computing) flows which are either managerially unacceptable or unrealistic.

$$R_{\kappa,k}^L \leq \sum_{\bar{o}=1}^{N_{\kappa}} (q_{\bar{o},k}^s) \leq R_{\kappa,k}^U \quad (12)$$

Where κ = identifier for a particular reach number; N_{κ} = number of cells in reach κ ; $R_{\kappa,k}^L, R_{\kappa,k}^U$ = lower and upper bounds on stream-aquifer interflow for reach κ , during stress period k , $[L^3T^{-1}]$.

3.2.8. Expressions Describing Flow Reduction

This constraint is used for situations in which a portion of a confined aquifer may become unconfined and unsaturated. This frequently occurs when pumping causes the piezometric surface to drop below the top of an aquifer layer.

- Piecewise linear flow-reduction constraint:

$$\begin{aligned}
 q^p_{\bar{o},k} &= cv_{i,j,l} (h_{i,j,l+1,k} - Top_{i,j,l+1}) & \text{for } h_{i,j,l+1,k} \leq Top_{i,j,l+1} \\
 q^p_{\bar{o},k} &= 0 & \text{for } h_{i,j,l+1,k} > Top_{i,j,l+1} \\
 cv_{i,j,l} &= \frac{\Delta x_i \Delta y_j}{\frac{\Delta z_{l+1}}{2 Kz_{i,j,l+1}} + \frac{\Delta z_l}{2 Kz_{i,j,l}}}
 \end{aligned} \tag{13}$$

- Nonlinear flow reduction constraint:

$$q^p_{\bar{o},k} = cv_{i,j,l} \min(h_{i,j,l+1,k} - Top_{i,j,l+1}, 0) \tag{14}$$

where $cv_{i,j,l}$ = vertical conductance [L^2T^{-1}]; $Top_{i,j,l+1}$ = top of aquifer layer $l+1$ in cell $i,j,l+1$, [L].

3.2.9. Expressions Describing Drain-aquifer Interflow

This constraint is intended to simulate drains that remove water at a rate proportional to the difference between the head in the aquifer and the head in the drain. If the water table is below the base of the drain, groundwater flows to the drain.

- Piecewise linear drain-aquifer interflow constraint:

$$\begin{aligned}
 q^d_{\bar{o},k} &= \gamma_{\bar{o},k} (h_{\bar{o},k} - d_{\bar{o}}) & \text{for } h_{\bar{o},k} \geq d_{\bar{o}} \\
 q^d_{\bar{o},k} &= 0 & \text{for } h_{\bar{o},k} < d_{\bar{o}}
 \end{aligned} \tag{15}$$

- Nonlinear drain-aquifer interflow constraint:

$$q^d_{\bar{o},k} = \gamma_{\bar{o},k} \max(h_{\bar{o},k} - d_{\bar{o}}, 0) \tag{16}$$

where $\gamma_{\bar{o},k}$ = hydraulic conductance of drain-aquifer interconnection, [L^2T^{-1}]; $d_{\bar{o}}$ = the drain elevation in cell \bar{o} , [L].

3.2.10. Monotonocity and Sustainability Constraint

This constraint insures that pumping increases monotonically (i.e., increases or remains the same, but never decreases). It also assures that the computed optimal pumping is sustainable.

$$g_{\bar{o},k-1} \leq g_{\bar{o},k} \leq g_{\bar{o}}^{ss} \quad (17)$$

where $g_{\bar{o}}^{ss}$ = an initially unknown steady groundwater pumping beyond the planning period, $[L^3T^{-1}]$. It is determined by the model during optimization using a set of steady-state flow constraints, in addition to the transient flow constraints of equation (2). and Knapp and Fienerman [1985] give a good rationale for the importance of sustained yield groundwater planning.

3.3. Bounds

These bounds are intended to enforce natural conditions, legal rights or management goals. They are placed on pumping, heads, and recharge across a single or the entire set of constant head-cells, respectively

$$g_{\bar{o},k}^L \leq g_{\bar{o},k} \leq g_{\bar{o},k}^U \quad (18)$$

$$h_{\bar{o},k}^L \leq h_{\bar{o},k} \leq h_{\bar{o},k}^U \quad (19)$$

$$(q_{\bar{o},k}^z)^L \leq q_{\bar{o},k}^z \leq (q_{\bar{o},k}^z)^U \quad (20)$$

where L and U denote lower and upper bounds on variables, O_c = total number of constant head cells on a boundary; QC_k^L and QC_k^U = lower and upper bounds on total lateral inflow to (outflow from) the aquifer through constant head cells along a boundary, $[L^3T^{-1}]$.

4. Solution Using Linear and Nonlinear Model Options

Above, both linear and nonlinear equations are used to represent processes in a nonlinear system. If only linear constraint equations are used, the resulting model is linear. If nonlinear constraints are used, the model is nonlinear. (Both the linear and nonlinear models are linear in transmissivity and dispersivities. Both assume these values are known (at the beginning of a cycle) for all stress periods, being computed using heads from initial conditions or a previous cycle.) How these two model forms are applied and why both are needed is discussed below.

4.1. *Linear Model*

When the linear model is applied to a nonlinear physical system, the model should be solved repeatedly (cycled) until convergence is achieved. Heads from the previous cycle are used to compute transmissivities and dispersivities, and to select the correct linear equations for Et, river-aquifer interflow, flow reduction, general head boundary and drain-aquifer-interflow. Advective transport is depicted linearly using (eq. 5) and the linear cyclical differencing approach described previously.

4.2. *Nonlinear Model*

When the nonlinear model is applied to a nonlinear system, Et, stream-aquifer interflow, drain-aquifer interflow, flow reduction, and seepage velocities are all represented by their nonlinear expressions. In the case of an unconfined aquifer, future transmissivity is still treated linearly. Transmissivity is the product of hydraulic conductivity and unknown future saturated thickness. Describing the system exactly would result in a highly nonlinear model that would be difficult to solve. In the model this nonlinearity is dealt with by recomputing transmissivities for all stress periods at the end of each cycle. Heads from the previous cycle are then used to compute transmissivities for the present cycle.

Concerning transport, only dispersivities are computed using velocities from the previous cycle. Advective transport is described nonlinearly, using equations 3 and 4. Cycling is still needed, because transmissivities and dispersivities are computed using heads from the previous cycle. Cycling is terminated when the maximum absolute value of differences in head for two consecutive cycles is less than a predetermined convergence criterion value.

5. USUEM's Integrated Modeling Structure

An integrated modeling approach was needed to permit efficient computation of optimal strategies for complex nonlinear study areas. Within the solution effort,

sometimes a linear formulation is needed, sometimes the nonlinear version is most suitable. In addition, there are two versions of both the linear and nonlinear models. The ability to expeditiously change from one form or version to the other is important. To achieve that, USUEM is interactive with the user and is modular.

USUEM consists of a series of modules. A module deals with input, output, a special action that should be taken by MINOS solver, or a specific feature of the hydrologic system (Et, stream-aquifer interflow, etc.) being simulated. The modules are designed to be as independent as possible. The modular structure is used to systematically prepare the objective function and all constraints and bounds needed for the optimization model described in section 3. This permits modifying or examining different options without affecting the rest of the model. Other options can be handled easily.

As previously mentioned there are two versions of both the linear and nonlinear model formulations. In the first version, Et, stream-aquifer interflow, general-head boundary condition, flow reduction, and drain-aquifer interflow are included as distinct variables in the flow equation (2). Additional expressions describing these processes exist separately in the model. In this 'partitioned' version, the model is written in a way such that each option is represented by a separate module containing the corresponding linear and nonlinear equations. The option's formulation can be changed in the corresponding module without making any modifications in the flow equation. This option facilitates future modifications and helps prevent mistakes. Also, this type of formulation is more flexible when adding new options. It should be used by new users and for small-scale problems.

The second version is considered a 'combined' version. In the combined version, all external head-dependent fluxes (Et, stream-aquifer interflow etc..) are replaced in the flow equation by the equations describing each as a function of head. Therefore, the only unknowns present in the modified flow equation are heads and pumping. No separate modules are called for Et, stream-aquifer interflow, general head boundary, and drains. All the options are represented by their corresponding equations within the expanded flow equation. Et, stream-aquifer interflow, general-head aquifer interflow, etc. are computed by postprocessor after the optimal solution is found.

Both combined and partitioned versions give the same results. The combined version requires fewer variables and fewer equations. It is faster and more suitable for large-scale problems.

5.1. *Integrated Approach Solution Technique*

The flow chart in Fig. 2 summarizes the methodology for computing optimal groundwater pumping strategies. Different modules and the order in which they are called are presented in Fig. 3.

After calling the modules requested by the user and selecting the version that will be used, both LP and the DNLP equations are compiled. Both are then ready for the user to apply as desired. The need for these two formulations is explained later.

5.2. *Switching between Linear and Nonlinear options*

USUEM permits the user to apply either the linear or the nonlinear model in any cycle. The ability to switch from one to the other can be useful and necessary if one of the options is experiencing numerical difficulties. The switching ability is an important feature of the integrated embedding modelling approach.

5.2.1. *Linear option*

Good reasons for using the linear model to solve groundwater management problems include solution speed and global optimality of solutions. As is well known, a linear model is easier to solve and generally solves more rapidly than a nonlinear model. We obtained essentially the same results from both models. Our comparisons involved several test cases and a range of initial guesses of optimal solutions for both models).

In some situations it is better to use the nonlinear instead of the linear form. In an initial optimization for a complicated physical system, if the initial guess (of the optimal solution) is not close to the optimal solution, a linear solver might declare the problem to be infeasible, even though a solution might exist. This results because in the LP formulation the equations describing Et, river and drain-aquifer interflow, and flow reduction are based on assumed heads. Even if those heads are the result of simulation by a reputable model (i.e., MODFLOW), computational tolerances can cause the redefined equations to be infeasible. In other words, preselection of linear equation segments excessively limits MINOS' freedom. This restriction can lead to an infeasible solution even though the problem could be optimized if the DNLP option were used.

Using the DNLP formulation can help because in that formulation, Et, river and drain-aquifer interflow and flow reduction are described by equations which are appropriate for the heads and pumping values being optimized. These fluxes are varied and adjusted within the model to get an optimal solution. In this study, some scenarios were run using both formulations. When infeasibilities were obtained using the LP formulation, the DNLP model was successful.

The linear formulation usually results in fewer numerical difficulties than the nonlinear model, once a feasible solution is obtained. In addition, it is easy to obtain convergence and optimality for problems derived by slightly modifying bounds in the original problem.

The LP model is useful for its ability to compute globally optimal solutions. The optimal solution to a linear problem is always globally optimal. However, it is difficult to prove that the optimal solution to a linear surrogate of a nonlinear problem is globally optimal. Similarly, it is not theoretically easy to prove that the solutions computed by DNLP model are globally optimal—especially in the presence of different processes that can be described by concave and convex functions according to parameters that might change from one cycle to another. However, it is possible to get feeling of the global optimality of a nonlinearly optimal solution by running the LP model using results from the nonlinear formulation. Our experience has been that both LP and DNLP models

developed by USUEM ultimately compute the same optimal strategies. This has involved several test cases and a wide range of different initial guesses (of the optimal strategy) for both models.

5.2.2. *Nonlinear option*

The nonlinear formulation better represents field conditions. To address the nonsmooth constraint equations of Et, river-aquifer interflow, etc., MINOS uses a special DNLP solver. This solver is designed for cases having discontinuous derivatives, in which Min and Max functions are used.

The DNLP model is sometimes better than the LP model for developing feasible solutions at the beginning of a series of optimizations. However, some effort should still be expended in developing good initial guesses of those optimal solutions. The time required for each model to develop an optimal solution is dependent on how good the initial guess is.

Once both LP and DNLP models are successfully computing optimal strategies, the DNLP model requires more CPU time.

6. Numerical Difficulties and Possible Solutions

Possible difficulties occurring when using the solution procedure are discussed below. They are presented to aid others in applying the embedding method to nonlinear groundwater management problems.

6.1. *Solver Declares Problem To Be Infeasible*

Several situations can cause this case:

One case exists if the number of infeasibilities is great (more than 5 infeasibilities for the Salt Lake study area). Model output should be analyzed to see where the infeasibilities are occurring. If the constraints and (or) bounds can be modified without too greatly weakening the model formulation and objective, the bounds on the infeasible variables should be relaxed and the model rerun. If bounds and constraints should not be modified, another initial guess should be tried. If many alternatives are unsuccessfully tried, one might conclude that the problem is infeasible under that formulation. That means that the modeler is trying to force the model to do something that is physically impossible to do.

A second case exists if the number of infeasibilities is small and the number of previous cycles is not great. If the LP solver is being used, switch to the DNLP solver. Usually an optimal solution is then obtained. This results because in the LP formulation the equations describing Et, river and drain-aquifer interflow, and flow reduction are based on previous heads. By that act, model choices are limited somewhat before optimization starts. That restriction can lead to an infeasible solution even though the

problem could be optimized if the DNLP option were used. Changing to a DNLP formulation can help because in that formulation, Et, river and drain-aquifer interflow and flow reduction are implicit or explicit variables and are more realistically determined within the optimization process. They are varied and adjusted within the model to get an optimal solution. In this study, some scenarios were run using both formulations. When the LP formulation yielded infeasibilities, the DNLP form was subsequently successful, even if it required several cycles. Ultimately, using the LP model after the DNLP model would also yield optimal solutions.

6.2. *Other Difficulties*

Some of the subsequent problems can be solved quickly. Others are more difficult to solve and require changes in the default MINOS options. Changes can be accomplished by editing a special file (**minos5.opt**). These options involve modifying some of the default parameters in the numerical methods used in MINOS. They are all described in the MINOS manual (Murtagh and Saunders, [1987]). From experience the following tips can help solve some of the problems dealing with embedding groundwater management models.

1. A common MINOS error message for this type of problems is the basis is structurally singular after two factorization attempts. This is usually the result of the numerical singularity in the basis. The option to be tried first is to change the Lu factor tolerance using MINOS options. Usually a value of 1 for both Lu factor tolerance and Lu update tolerance gives satisfactory results. Running the LP formulation instead of the DNLP can also be helpful.

2. Finally, the error message the superbasics limit is too small is used when the problem is more nonlinear than anticipated. From experience, it is recommended that one try the LP formulation.

Other suggestions about MINOS's options can be found in users's guide. It is very important to be familiar with these options and have an idea about the structure of the model (density and sparsity of the Jacobian matrix). Also, a good initial guess is very important. If an initial guess is not provided, MINOS uses zero or the closest bound to zero as an initial guess. It is also important to provide reasonable bounds. They limit the search to the feasible region, and prevent undefined operations. In addition, sometimes a well formulated problem is infeasible only because of errors in input data. Such mistakes can be corrected or avoided if the input listing is checked carefully.

7. **Summary and Conclusions**

7.1. *Summary*

Presented is an integrated methodology for optimizing ground-water yield planning in nonlinear multilayer aquifer systems having dispersed contamination. The

methodology utilizes the embedding approach to represent flow and transport within an optimization model. The methodology enhances capabilities to address nonlinear problems and overcomes difficulties previously associated with using the embedding methods. The result is suitable for optimizing large scale reconnaissance level planning.

This methodology is incorporated within the USUEM model, which contains embedded implicit finite difference quasi-three-dimensional unsteady saturated flow equations. These differentiate between the following flow processes: evapotranspiration (E_t), stream-aquifer interflow, discharge from wells and drains, recharge, flow reduction due to dewatering of previously confined aquifers, and boundary conditions. USUEM also contains embedded finite element two-dimensional saturated steady and transient transport equations.

To overcome previously reported weaknesses (difficulty in computing feasible solutions, processing time and memory requirements), and to make the method applicable to more complex nonlinear problems, the methodology includes the following.

- Both linear and nonlinear models are used to represent the same problem.
 - To aid speed of processing, fully linear versions of flow and transport are used. This includes a new development, the cyclical linear differencing method for representing transient advective transport in an optimization model. This method permits optimizing unsteady pumping and transient flow even while contaminated water is being extracted.
 - To aid the ability to find feasible solutions, nonlinear versions of flow and transport equations are used (transmissivity and dispersivity are still treated linearly by using the heads and velocities of a previous cycle. This is the first report of computing concentrations using a fully embedded nonlinear finite element advective transport equation for an unknown transient flow field in which contaminated groundwater is being extracted. Also newly reported is the use of discontinuous nonlinear programming to represent flow processes having nonsmooth piecewise functions and discontinuous derivatives (E_t , stream-aquifer interflow, flow from drains.)
- To aid assessment of solution global optimality, both linear and nonlinear versions are used and the results are compared with each other. The optimal solution from the nonlinear model can be used as the initial guess for solving the linear model, or vice versa.
- To improve the ability to identify feasible solutions or to speed processing, respectively, either a partitioned or a combined form of the flow equation can be used for either the linear or the nonlinear model.
 - To aid the ability to find feasible solutions by identifying flow processes causing constraint violations, a version in which flow processes are partitioned into several different equations is used. In addition to the common finite difference equation for saturated flow, this version has separate equations, and variables, defining E_t , stream-aquifer interflow, flow reduction and flow from drains.
 - To speed processing and reduce computer memory requirements a version using a combined flow equation is used. It has only one flow equation, which includes all ground water flow processes (flow between cells, E_t , etc.) and has only

pumping and head as variables. In this version all the external flow processes are represented in terms of head.

- To avoid making the problems too nonlinear and difficult to solve, transmissivity and contaminant dispersion are treated as knowns in each optimization. This requires the use of cycling (performing successive optimizations). The cycling process is as follows.

1. Based on expected or optimal water management, assume or compute initial and future values of transmissivity and dispersion.
2. Utilize the expected transmissivity and dispersion values within the optimization model to compute an optimal strategy.
3. Compare the optimal strategy and strategy results (i.e. heads) with those used to compute transmissivity and dispersion in step 1. If there is insignificant difference, stop. Otherwise, return to 1 and cycle.

- To permit rapid use of all the above features, USUEM is modular and interactive. This permits easy cycling between successive optimizations, and easy switching between linear and nonlinear versions between cycles.

- To integrate groundwater yield planning with management of dispersed (nonpoint source) contamination, the multiobjective function uses the weighting method. The model can:

1. maximize groundwater mining
2. maximize sustainable groundwater extraction
3. minimize the degree to which future groundwater concentrations at control nodes exceed target concentrations.
4. perform combinations of 1 and 3 or 2 and 3.

The methodology is most applicable for the same sort of situation the embedding approach has historically been most useful for--reconnaissance-scale sustained groundwater yield planning where: (1) cells are relatively large, and (2) proportions of cells requiring head constraint or containing pumping as a decision variable are great. It is assumed that each cell might contain many wells and that the head and concentration computed for the center of a cell is adequately representative for such coarse planning.

7.2. *Conclusions*

The embedding technique can be adapted to optimize groundwater planning for more complicated problems than reported previously. This is done by integrating use and coordinating use of both linear and nonlinear forms of flow and transport equations. The integrated procedure can address steady-state and transient groundwater quantity and quality management studies for complex nonlinear multi-layer aquifer systems. (A companion paper illustrates its application for large-scale, long-term planning.)

The integrated approach makes it easier to develop solutions than previously. Utilizing both linear and nonlinear model forms permits successful optimization when using only one form would not. Selectively switching from one form to the other decreases the time and difficulty spent in obtaining feasible and optimal solutions for nonlinear aquifer systems.

The integrated model computes optimal strategies that will satisfy future management goals in terms of heads, flows and concentrations. It can maximize sustainable groundwater pumping while causing the attainment of target groundwater contaminant concentrations at pre-specified control locations.

The model should be most useful for sustained yield groundwater planning in areas typified by: (1) large cells, each possibly containing many wells, (2) large proportion of cells contain pumping as a decision variable or require head constraint, and (3) significant variable head-affected external fluxes (E_t , etc.), or (4) dispersed groundwater contamination requiring management.

FIGURE 1. Description of a Cycle.

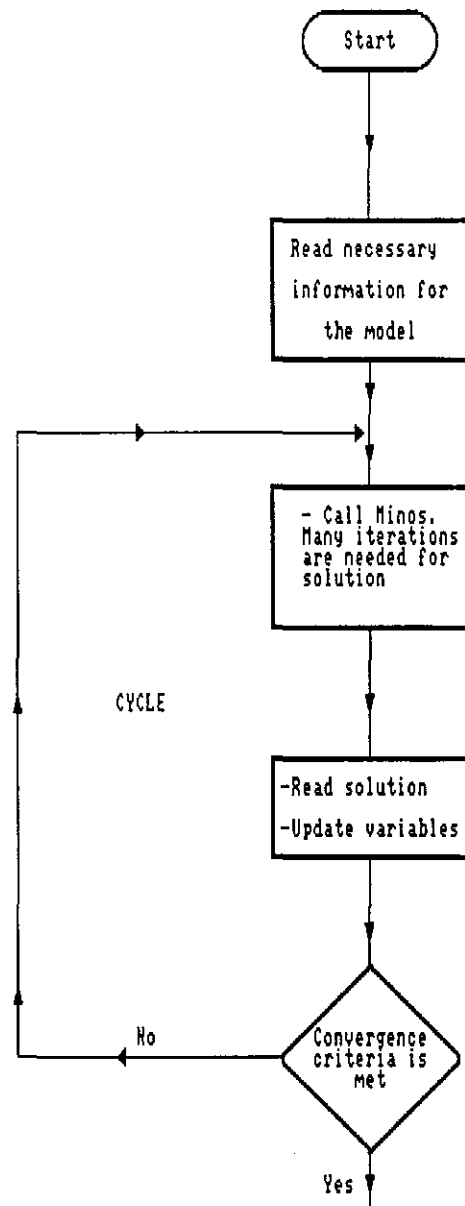


FIGURE 2. Man/Machine Decision Tree for Computing Optimal Solution Using USUGWM.

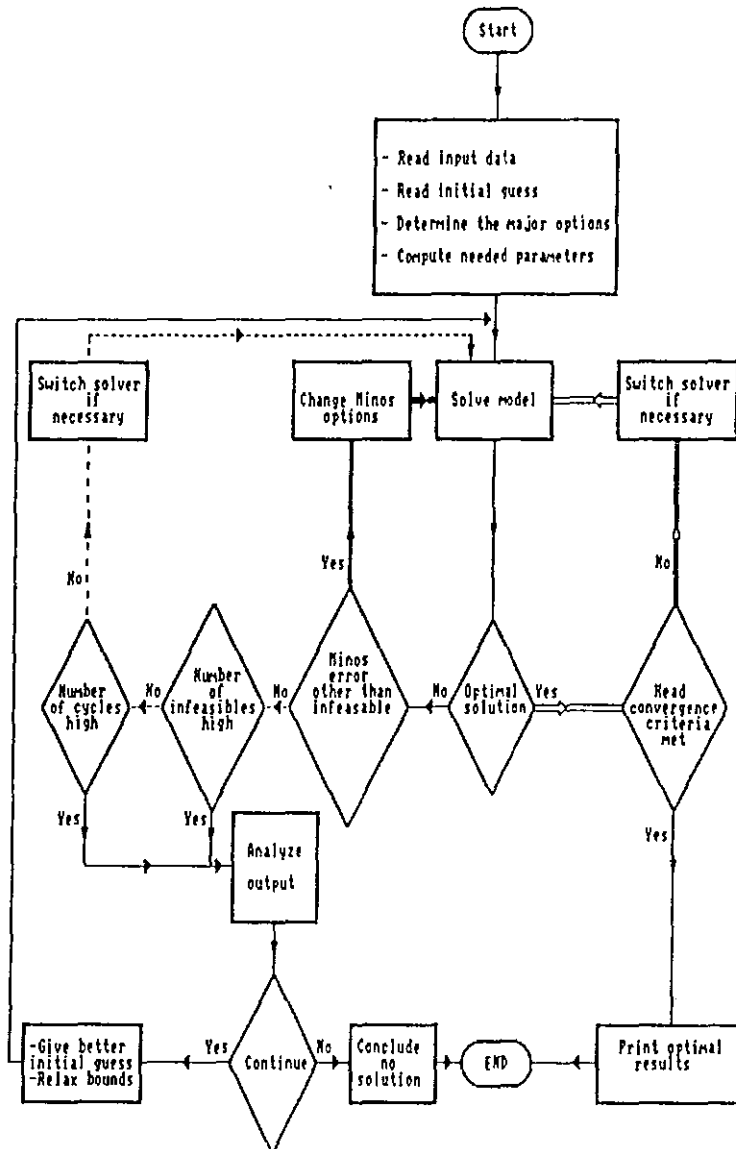
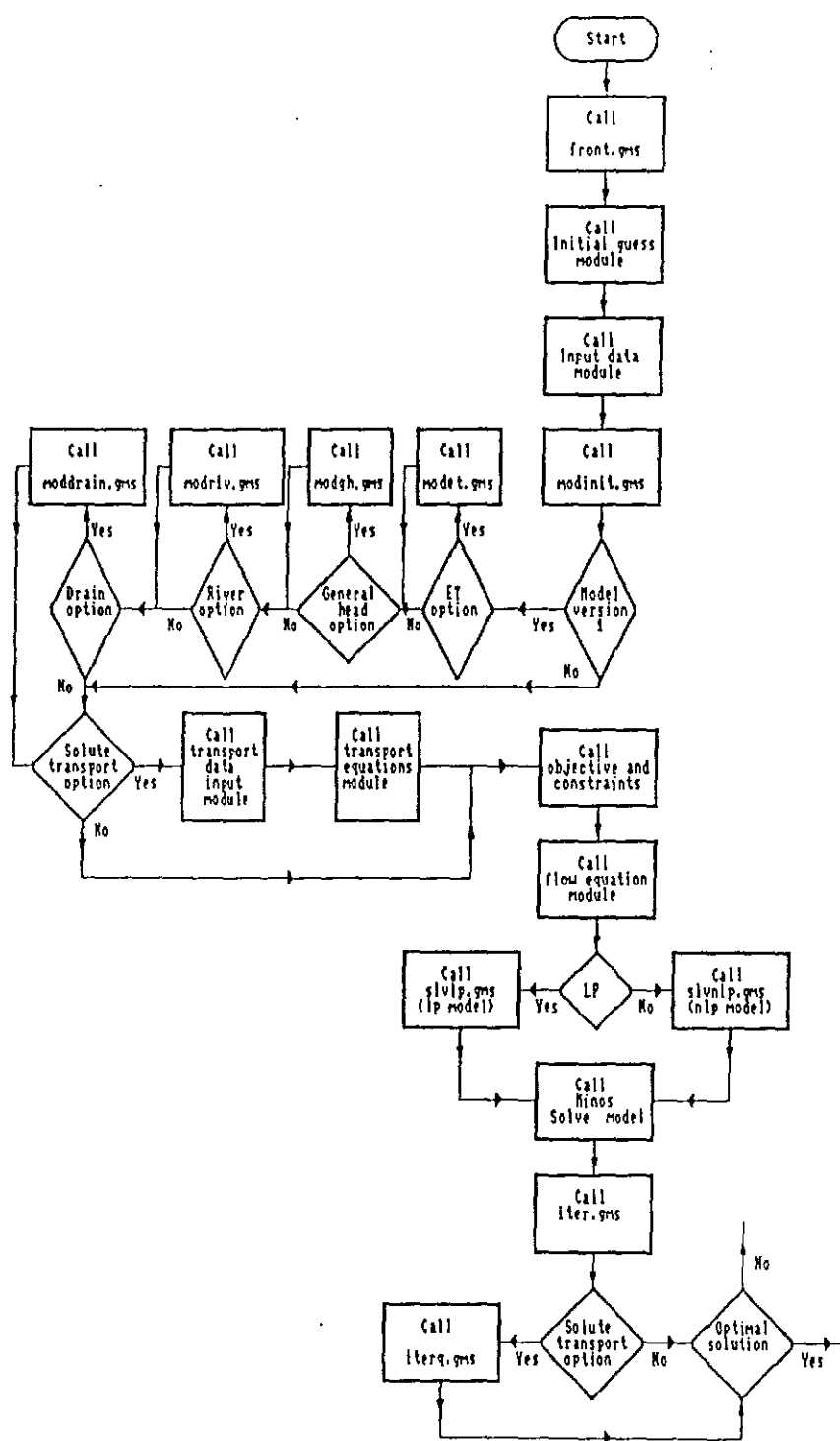


FIGURE 3. Overview of Data Input, Model Construction, Solution Process, and Modules Called.



Notation

b	saturated thickness of the aquifer	[L]
B_n	column vector associated with the boundaries and sources or sinks term	[ML ³ T ⁻¹]
$B_{\bar{o}}$	bottom of the river in cell \bar{o}	[L]
c	concentration of the dissolved chemical species	[ML ⁻³]
$Cv_{i,j,l}$	vertical conductance	[L ² T ⁻¹]
c^*	solute concentration in the source fluid	[ML ⁻³]
$c_{nq,kq}^{\text{target}}$	target concentration at node nq by the end of time step kq	[ML ⁻³]
$c_{nq,kq}^+$	excess concentration with respect to target concentration for node nq by the end of time step kq	[ML ⁻³]
$c_{nq,kq}^-$	amount by which the simulated concentration is below the target concentration in node nq by the end of time step kq	[ML ⁻³]
D_{ij}	coefficient of hydrodynamic dispersion	[L ² T ⁻¹]
$d_{\bar{o}}$	the drain elevation in cell \bar{o}	[L]
$ds_{\bar{o}}$	extinction depth in cell \bar{o}	[L]
e	a designator identifying one of the total of E elements	none
$E_{\bar{o}}$	potential evapotranspiration in cell \bar{o}	[L]
$g_{\omega,k}$	pumping (+) from cell ω , during stress period k	[L ³ T ⁻¹]
h	potentiometric head	[L]
$hc_{\bar{o},k}$	potentiometric head for the general-head boundary in cell \bar{o}	[L]

hs_{ϕ}	potentiometric surface elevation below which the evapotranspiration rate begins to decrease	[L]
$h_{\phi,1}$	head in layer 1 and cell ϕ of coordinates (i,j) where water is of poor quality	[L]
K_{ij}	hydraulic conductivity	[LT ⁻¹]
kq	time step used for water quality simulation	[T]
$l(e)$	the length of the rectangular element e	[L]
m and n	designator identifying individual nodes from among the N total finite-element nodes where concentrations are to be computed	none
$\max(r,s)$	function equalling the greater of the numerical values of equations denoted by r and s	
$\min(r,s)$	function equalling the lesser of the numerical values of equations denoted by r and s	
NQ	total number of nodes where water quality control is required	none
$N\kappa$	number of cells in reach κ	none
Oc	total number of constant head cells on a boundary	none
\bar{o}	cell (i,j,l)	none
QC_k^L	lower bound on total recharge through constant head cells	[L ³ T ⁻¹]
QC_k^U	upper bound on total recharges through constant head cells	[L ³ T ⁻¹]
$q_{\bar{o},k}^b$	known horizontal flow across the boundary	[L ³ T ⁻¹]
$q_{\bar{o},k}^c$	saturated flow between the aquifer and the general head boundary cells	[L ³ T ⁻¹]
$q_{\bar{o},k}^d$	flow from the aquifer to drains (+)	[L ³ T ⁻¹]

$q_{\bar{o},k}^p$	reduction in vertical flow between cells in layer 1 and the lower layer 1+1	$[L^3T^{-1}]$
$q_{\bar{o},k}^s$	flow between the aquifer and streams	$[L^3T^{-1}]$
$q_{\bar{o},k}^l$	distributed evapotranspiration	$[L^3T^{-1}]$
$q_{\bar{o},k}^z$	horizontal flow across a boundary	$[L^3T^{-1}]$
$R_{\kappa,k}^L$	lower bound on stream-aquifer interflow for reach κ , during stress period k	$[L^3T^{-1}]$
$R_{\kappa,k}^U$	upper bounds on stream-aquifer interflow for reach κ , during stress period k	$[L^3T^{-1}]$
S	specific yield for unconfined aquifer or storage coefficient for confined aquifer	none
t	time	$[T]$
$Top_{i,j,l+1}$	top of aquifer layer 1+1 in cell $i,j,l+1$	$[L]$
T_{xx}	transmissivities along x direction	$[L^2T^{-1}]$
T_{yy}	transmissivities along y direction	$[L^2T^{-1}]$
T_{zz}	transmissivities along z direction	$[L^2T^{-1}]$
$ V $	magnitude of the seepage velocity	$[LT^{-1}]$
V_x	seepage velocities in the x direction	$[LT^{-1}]$
V_y	seepage velocities in the y direction	$[LT^{-1}]$
W	volume flux per unit area	$[LT^{-1}]$
wc	weighting factor associated with quality control	$[L^6M^4T^{-4}]$
$w(e)$	the width of the rectangular element e	$[L]$
$[A_D]^*$	the influence coefficient matrices associated with the dispersive term in the transport equation	$[L^{-2}]$

$[A_s]^e$	the influence coefficient matrices associated with the source sink term in the transport equation	$[L^{-2}]$
$[A_t]^e$	the influence coefficient matrices associated with the time term in the transport equation	none
$[E_v^*]^e$	the influence coefficient matrices associated with the centroid velocities term in the transport equation	$[L^{-2}]$
$\langle V_x \rangle^e$	the centroid values of seepage velocities in the x direction for element e	$[L^2T^{-1}]$
$\langle V_y \rangle^e$	the centroid values of seepage velocities in the y direction for element e	$[L^{-2}]$
σ^u	resistance of the upper confining layer	$[T]$
σ^l	resistance of lower confining layer	$[T]$
ε	effective porosity of the aquifer	none
α_L	longitudinal dispersivity	$[L]$
α_T	transverse dispersivity	$[L]$
Ω	total number of pumping cells in the study area	none
Δt_k	duration of stress period k	$[T]$
Δt_{kq}	duration of the time step kq, a fraction of Δt_k	$[T]$
Δx_j	cell size in x direction located in row i	$[L]$
Δy_i	cell size in y direction located in column j	$[L]$
Δz_l	cell size in z direction located in column l	$[L]$
$\Gamma_{\bar{o}}$	hydraulic conductance of the stream-aquifer interconnection	$[L^2T^{-1}]$
$\sigma_{\bar{o},k}$	elevation of the free water surface in the river	$[L]$

κ	identifier for a particular reach number	none
$\gamma_{\bar{o},k}$	hydraulic conductance of drain-aquifer interconnection	$[L^2T^{-1}]$

References

- Aguado, E. and Remson, I. 1974. "Ground-water hydraulics in aquifer management," Journal of Hydraulics Division, ASCE 100(HY1):103-119.
- Ahfeld, D.P., Mulvey, J.M., and Pinder, G.F. 1986. "Designing optimal strategies for contaminated groundwater remediation," Advances in Water Resources 9(2):77-84.
- Ahfeld, D.P., Mulvey, J.M., Pinder, G.F., and Wood, E.F. 1988. " Contaminated groundwater remediation design using simulation, optimization and sensitivity theory," Water Resources Research 24(3):431-442.
- Ahfeld, D.P. 1990. "Two-stage ground-water remediation," Water Resources Planning and Management 116(4):517-529.
- Cantiller, R.A., Richard, C.P., and Hossein, A. 1988. "Optimal conjunctive use-sustained yield pumping analysis for eastern Arkansas," Misc. Pub. No. 40, Arkansas Water Resources Research Center, Univ. of Arkansas, Fayetteville, Arkansas, and IIC Report IIC-88/2:126.
- Culver, T.B., and Shoemaker, C.A. 1992. " Dynamic optimal control for groundwater remediation with flexible management periods," Water Resources Research 28(3):629-641.
- Danskin, W.R., and Gorelick, S. M. 1985. "A policy system using controlled stream recharge," Water Resources Research 21(11):1731-1747.
- Datta, B., and Peralta, R.C. 1986. "Interactive computer graphics-based multiobjective decision-making for groundwater management," Agricultural Water Management (11):91-116.
- Dougherty, D.E. and Marryott, R.A. 1991. "Optimal Groundwater Management 1. Simulated annealing," Water Resources Research 27(10):2493-2508.
- Elango, K., and Rouve, G 1980. "Aquifers: Finite-element linear programming model," Journal of Hydraulics Division, ASCE 106(HY10):1641-1658.
- Evans, B. and Remson, I. 1982. "Closure : Ground-water management with fixed charges," Water Resources Planning and Management 108(2):237
- Gorelick, S.M. 1983. "A review of distributed parameters groundwater management modeling methods," Water Resources Research 19(2):305-319.

Gorelick, S.M. and Voss, C.I. 1984. "Aquifer reclamation design: the use of contaminant transport simulation combined with nonlinear programming," Water Resources Research 20(4):415-427.

Huyakorn, P.S., Jones, B.G., and Anderson, P.F. 1986. " Finite-element algorithms for simulating three-dimensional groundwater flow and solute transport in multilayer aquifer," Water Resources Research 22(3):361-374.

Knapp K. C. and Fienerman, E. 1985. "The optimal steady-state in groundwater management," Water Resources Bulletin 21(6):967-975.

McDonald, M.G. and Harbaugh, A.W. 1984. "A modular three-dimensional finite-difference ground-water flow model," U.S. Geological Survey Open File Report 83-875, Book 6, Modeling techniques, Washington, DC.

Molz, F.J. and Bell, L.C. 1977. "Head gradient control in aquifers used for fluid storage," Water Resources Research 13(4):253-260.

Murtagh, B.A. and Saunders, M.A. 1987. "MINOS 5.1 User's Guide," Report SOL 83-20R, December 1983, revised January 1987, Stanford University.

Peralta, R.C., and Killian, P.J. 1985. "Optimal regional potentiometric surface design: Least cost water supply/sustained groundwater yield," Transactions of the ASAE 28(4):1098-1107.

Peralta, R.C. and Killian, P.J. 1987. "Decision support for optimal regional groundwater management strategy modification," American Society of Agricultural Engineers 30(2):400-410.

Peralta, R.C. and Datta, B. 1990. "Reconnaissance-level alternative optimal groundwater use strategies," Water Resources Planning and Management, ASCE 116(5):676-692.

Voss, C.I. 1984. "A finite element simulation model for saturated-unsaturated fluid density dependant groundwater flow with energy or chemically reactive solute transport," U.S. Geological Survey, Reston, Virginia -410.

Willis, R. 1979. "A planning model for the management of groundwater quality," Water Resources Research 15(6):1305-1312.

Willis, R. and Jones, L. 1987. "Optimization of unconfined groundwater systems: A differential dynamic programming algorithm," Geological Society of India 29(1):83-104.

Willis, R., Finny A. B., and Zhang, D. 1989. "Water Resources management in north China plain," Journal of Water Resources Planning and Management 115(5):598-615.

Yazdanian, A. and Peralta, R. 1986. "Maintaining target groundwater levels using goal-programming: linear and quadratic methods. Transactions of the American Society of Agricultural Engineers 29(4):995-1004.

Yazicigil, H. and Rasheeduddin, M. 1987. "Optimization model for groundwater management in multi-aquifer systems," Water Resources Planning and Management 113(2):257-275.